# Effective Estimation of Ligand-Binding Affinity using Biased Sampling Method

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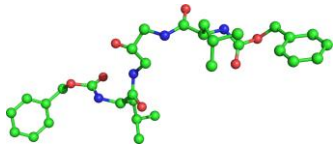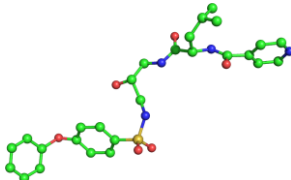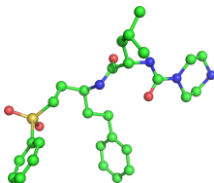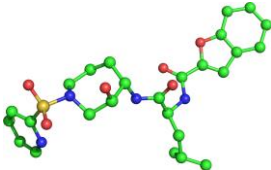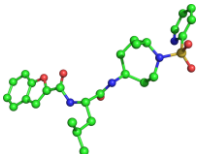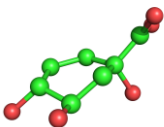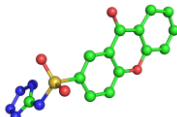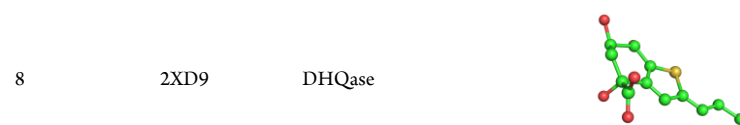
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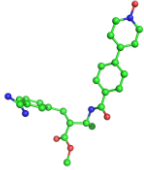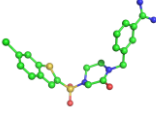[b]Faculty of Applied Sciences, Ton Duc Thang University, Ho Chi Minh City, Vietnam,
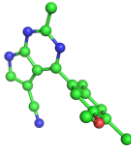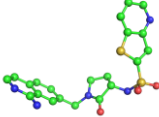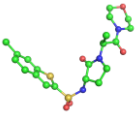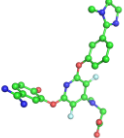
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**Table S1.** List of ligands and their structure

| N# | Complexes | Protein | Ligand |
|----|-----------|---------|--------|
| 1 | 1AU0 | CTSK |  |
| 2 | 1AU2 | CTSK |  |
| 3 | 1MEM | CTSK |  |
| 4 | 1NLJ | CTSK |  |
| 5 | 2FTD | CTSK |  |
| 6 | 1GU1 | DHQase |  |
| 7 | 2C4W | DHQase |  |

| | | | |
|---|---|---|---|
| 8 | 2XD9 | DHQase | |
| 9 | 2Y71 | DHQase | |
| 10 | 4B60 | DHQase | |
| 11 | 3K99 | HSP90 | |
| 12 | 3QDD | HSP90 | |
| 13 | 3R4M | HSP90 | |
| 14 | 3R4N | HSP90 | |

| 15 | 3RLQ | HSP90 | |

| 16 | 1F0R | FXa | |

| 17 | 1KSN | FXa | |

| 18 | 1NFU | FXa | |

| 19 | 2J34 | FXa | |

| 20 | 1FJS | FXa | |
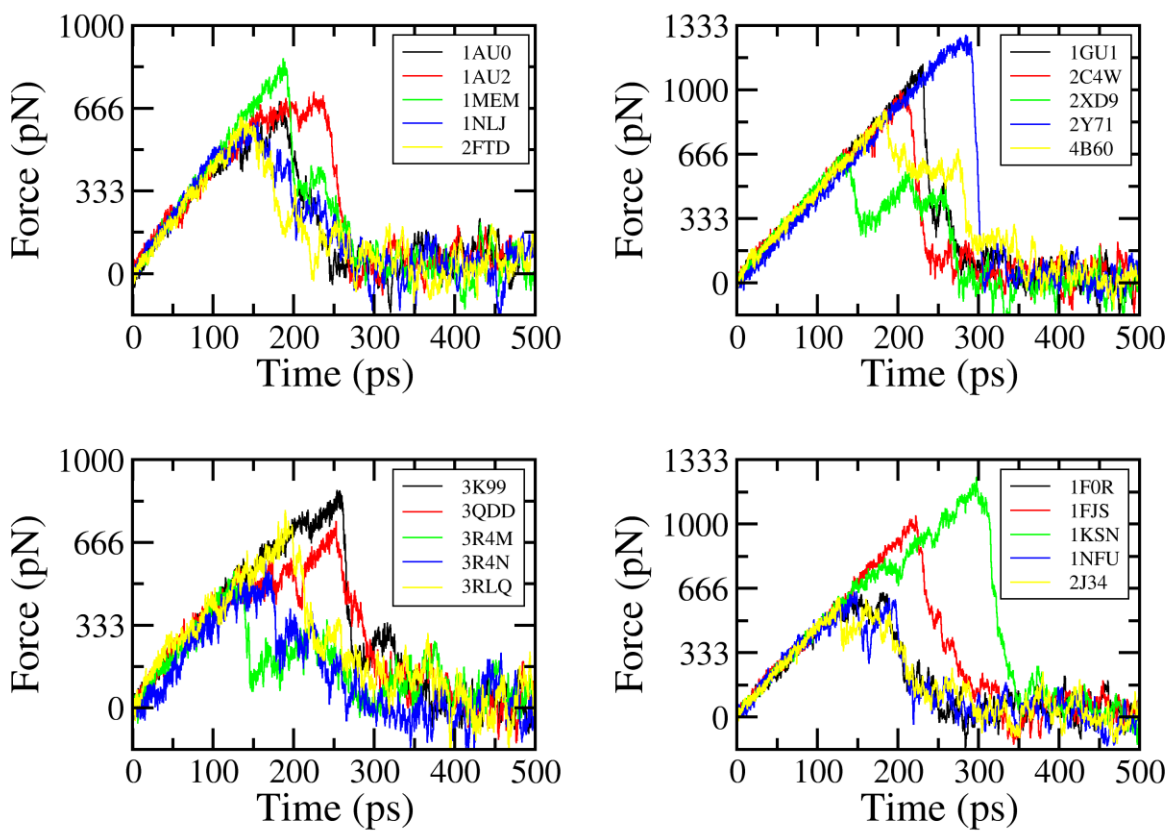
**Figure S1.** The recorded values of pulling force over FPL simulations
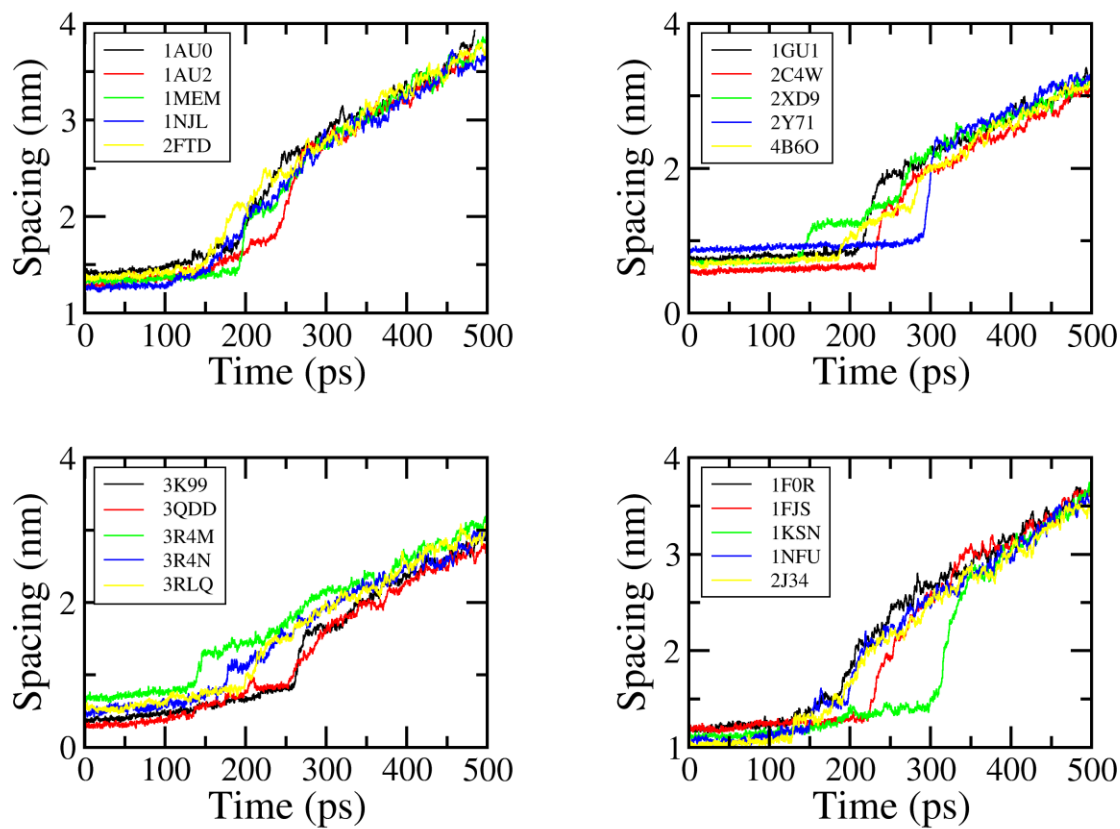
**Figure S2.** The displacement of the ligand center of mass during FPL simulations